

Isoamyl ether
544-01-4 | DTXSID8052198

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.23

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

Image not found

Isoamyl ether

Measured: 4.25

Predicted: 4.23

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Propane, 1,1'-oxybis[2-methyl-

Measured: 2.78

Predicted: 2.92

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Nonane

Measured: 5.65

Predicted: 5.44

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Octane

Measured: 5.18

Predicted: 5.05

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Butyl ether

Measured: 3.21

Predicted: 2.99